DRAFT

LA-UR-00-5034

*Approved for public release;
distribution is unlimited.*

Title: Workshop on Statistical Approaches for the Evaluation of Complex Computer Models

Author(s): Richard A. Berk, Peter Bickel, Katherine Campbell, Robert Fovell, Sallie Keller-McNulty, Elizabeth Kelly, Rodman Linn, Byungkyu Park, Alan Perelson, Nagui Rouphail, Jerome Sacks, and Frederic Schoenberg

Submitted to: Statistical Science

DRAFT

Workshop on Statistical Approaches for the Evaluation of Complex Computer Models

Richard A. Berk, Peter Bickel, Katherine Campbell, Robert Fovell, Sallie Keller-McNulty, Elizabeth Kelly, Rodman Linn, Byungkyu Park, Alan Perelson, Nagui Rouphail, Jerome Sacks, and Frederic Schoenberg

Abstract. As decision- and policy-makers come to rely increasingly on estimates and simulations produced by computerized models of the world, in areas as diverse as climate prediction, transportation planning, economic policy and civil engineering, the need for objective evaluation of the accuracy and utility of such models likewise becomes more urgent. This article summarizes a two-day workshop that took place in Santa Fe, New Mexico in December 1999, whose focus was the evaluation of complex computer models. Approximately half of the workshop was taken up with formal presentation of four computer models by their creators, each paired with an initial assessment by a statistician. These prepared papers are presented, in shortened form, in Section 3 of this paper. The remainder of the workshop was devoted to introductory and summary comments, short contributed descriptions of related models, and a great deal of floor discussion, which was recorded by assigned rapporteurs. These are presented in Sections 2 and 4 in the paper. In the introductory and concluding sections we attempt to summarize the progress made by the workshop and suggest next steps.

Key words and phrases: model accuracy, model evaluation, model validation, uncertainty analysis, computer experiments, statistically equivalent models, model-based decisions

1. INTRODUCTION

Complex computer models for the simulation of real world systems are used pervasively in scientific research, and there are increasing demands for these models to support policy- and decision-making. The foundations for such models range from the best available scientific theory ("structurally valid models" in the terminology of Zeigler [1976]) to empirical observation, common sense, and computational convenience. Frequently, they are assembled by coupling a number of simpler models. A key question is how good these complex computer models really are for their intended purposes. A subsequent question is how to make the models better.

Such issues prompted the National Academy of Sciences (NAS) Committee on Applied and Theoretical Statistics (CATS) to initiate planning for and eventually co-host a workshop on computer model evaluation[1] with Los Alamos National Laboratory and the National Institute of Statistical Sciences. The goal of the workshop was to bring modelers, applied mathematicians, and statisticians together to consider the role statistical concepts and tools could play in these evaluations.

The workshop drew a cross-section of nearly 100 scientists from academia, industry, and government. Participants included modelers from the physical and biological sciences, applied mathematicians, and statisticians, with nearly half the participants being modelers with subject-matter expertise. Participants were asked to focus on four key questions throughout the workshop:

(1) **What do we mean by model evaluation?** While there is no dispute that computer models should usefully approximate the real-world phenomena at issue, there is often lack of clarity about what aspects of the approximation are important within the proposed research or policy context. Moreover, under the rubric of "model evaluation" can be found everything from eyeball assessments to rigorous and formal characterizations, with some judgments derived from an aggregate measure of fit and others from a focus on certain key features of model output.

(2) **What makes model evaluation difficult?** There is a daunting abundance of complications: poor calibration; lack of data as "ground truth;" misalignment of temporal and spatial scales between the model output and available data; costs of both simulation and data replicates; large numbers of free parameters; and variability in modeled phenomena, data, and in the simulation itself.

(3) **What strategies for model evaluation can be employed?** Model evaluations have been undertaken for decades by subject-area experts, and there is, at the very least, extensive lore about how this should be done. An important goal of the workshop was to collect and organize this lore and then suggest other possible model evaluation strategies.

(4) **What is the role of statistical concepts and tools, and where are the statistical gaps?** There are a number of model evaluation concerns that can already be addressed by (computationally feasible) statistical methods. But an important task of the workshop was to systematically reconsider these methods in the context of particular model evaluation strategies: for instance,

[1] Workshop on Statistical Approaches for the Evaluation of Complex Computer Models was held December 3-4, 1999.

a method that may work well for comparing computer model output to data may not work well for comparing two sets of computer model output. A related task was to document serious gaps between what may be needed for model evaluation and what statisticians can currently provide.

The workshop began with a keynote address by Dr. William Press, the Deputy Director for Science, Technology, and Programs at Los Alamos National Laboratory (summarized in Section 2), the goal of which was to help frame the issues. This was followed by four sessions, each focused on a model drawn from a different scientific application:

- Meteorology
- Wildfire Control
- Transportation Planning
- Immune System Function

In each session, an overview of the computer model was provided by a subject-area scientist, followed by a statistical presentation discussing model evaluation approaches and problems in the context of the specific application model. These presentations laid the foundation for extensive discussion from the floor. Each session ended with a rapporteur placing that discussion in the context of the four workshop questions. The presentations are in Section 3; the discussions and rapporteur syntheses are presented in Section 4. Section 5 revisits the central themes of the workshop and provides a more complete discussion of important questions identified during the workshop (questions needing statisticians' attention), and offers suggestions about how progress might be made.

2. KEYNOTE ADDRESS: A TAXONOMY OF MODELS

Dr. William Press[2], Los Alamos National Laboratory (LANL) Deputy Director for Science and Technology, gave the keynote address. In the address Press proposed the following taxonomy of computer model types:

[2] Before coming to LANL in 1998, Press was Professor of Astronomy and Physics at Harvard University, and a member of the Theoretical Astrophysics group of the Harvard-Smithsonian Center for Astrophysics. Press has long been interested in computer modeling and simulation. He is the co-author and co-maintainer of the Numerical Recipes series of books on scientific computer programming. Press served on the NAS National Research Council (NRC) Computer Science and Telecommunications Board from 1991 to 1996, chaired the NAS/NRC Panel on Theory and Computation, Astronomy and Astrophysics Survey Committee from 1998 to 2000, and is currently the co-chair of the NAS/NRC Commission on Physical Sciences, Mathematics, and Applications.

1. “Accurate” models of deterministic physical phenomena with “accurate” input conditions
2. “Accurate” models of deterministic physical phenomena with “statistically accurate” input conditions
3. “Statistically accurate” models of non-deterministic physical phenomena
4. “Accurate” or “Statistically Accurate” models of emergent physical phenomena
5. “Phenomenologically Accurate” models that are not even statistically accurate
6. “Phenomenologically Interesting” models
7. “Video games” as models

Press noted that model evaluation requirements and issues vary depending on the model type. Accurate deterministic models (types 1&2) are models where the physics is well understood. He gave as examples static civil engineering models of bridges and dams, weapons codes, and “well-behaved” hydrodynamics models. He noted that for these models a single model run could be compared to data, using an appropriate norm. Classic issues associated with these models include whether all the physics is captured in the model, the effects of truncation vs. round-off errors, and the choice of what numerical model output to compare to data. He noted that where the input quantities are inherently stochastic or poorly known (type 2) there is also an issue of how to quantify model uncertainty from this source.

Statistically Accurate Models (type 3) include those treating innately statistical phenomenon, classical chaos, and having unknown initial conditions. Examples include turbulent fluid phenomena and climate models. These models might be conceptually deterministic, but for ensembles, not individual realizations. However, it is generally computationally impractical to make many runs. Press suggested that a theory of sparse Monte Carlo simulations might be useful. He identified additional issues in this setting, including how to determine which runs to make and how to establish metrics for evaluation both for model-to-model and model-to-data comparisons. In particular, how might we formalize the typical “eyeball” comparisons between model and data?

Emergent Models (type 4) capture the desired macro-phenomenology by describing an underlying micro-phenomenology that results in the desired phenomena. “Emergent” refers to the appearance of phenomena in the modeled system that are “neither explicitly represented in the system's elementary components or their couplings nor in the system's initial and boundary conditions.” [Reference: Das, R. Emergent computation in cellular automata.

http://cnls.lanl.gov/Highlights/1998-10/html/October_98.html]. These models need not look like "real physics." Examples include statistical mechanics, smooth particle hydrodynamics, cellular automata hydrodynamic, and traffic flow modeling. Press warned that there is no meta-theory of emergence and using these models may leave one vulnerable to self-deception.

Phenomenological Models (types 5 and 6) capture qualitatively identifiable phenomena, e.g. turbulent intermittency, traffic jams and epidemics. These models can be "inaccurate" in almost any statistical sense, yet be extremely useful. They can be used to train humans who can then quickly adjust to the actual phenomenology (e.g., fire fighters, who must make decisions about when to withdraw from an area). Issues for these models include how to map "fields of data" into "phenomena" or "events" and how to summarize the behavior (deterministic or statistical) of these phenomena.

Press concluded by suggesting a "space of models" and proposing a calculus for this space. He maintained that we seem to have an intuitive idea of such a space: codes can include *more* or *less* physics, models can be more *overlapping* or more *independent*, and we can envision a nested sequence of finer zoned codes. Press noted that intuitively we have the idea that a model result can be validated by *sampling* over the space of models and that when *different* codes agree, then they are both more likely to be accurate. He also noted that the more physics added, the more trustworthy the answer; ultimately, if we could compute "like nature" we would have the right answer. The claim of "the more physics, the more trustworthy" was actually disputed by the wildfire modeler and others in later sessions.

3. FOUR CONTEXTS for NUMERICAL MODELS

3.1 Mesoscale Modeling of Storm Events

3.1.1 The Scientific Problem and the Model
Presenter: Robert Fovell, University of California at Los Angeles

For the practice of atmospheric science, computer simulation models have become a key element in a wide variety of scientific and policy-related research. Applications can range in scale from particular chemical reactions to the climate of the entire earth. This presentation addressed mesoscale modeling of precipitation events in the Los Angeles Basin. The goal of the simulation was to provide model output, including but not limited to precipitation data, to be used as input to hydrological models for the investigation of streamflow and runoff in the region. As part of a computer model evaluation, it was decided to compare model output to data from one particularly strong precipitation event that occurred on 7-8 February 1993.

The computer model employed is known as MM5, or Mesoscale Model Version 5, a joint effort of the National Center for Atmospheric Research (NCAR) and Penn State University. MM5 is initialized using atmospheric observations and solves the equations governing physical, thermodynamic and microphysical processes within a three-dimensional domain that is subdivided into grid volumes. MM5 is a very complex modeling system. It includes many parameterizations that attempt to represent processes rendered unresolvable owing to temporal or spatial resolution limitations, such as the generation and dissipation of small turbulent eddies or the aggregation of cloud droplets into raindrops. To view graphical output from MM5 including annimated visualizations see http://www.scd.ucar.edu/vets/vg/Severegallery.html.

Precipitation fallout can be quite variable across the region, with the largest totals often recorded in the vicinity of mountain slopes. Therefore, accurate predictions of precipitation fallout depend upon an adequate representation of local orography, and this demands high spatial resolution. On the other hand, accurate handling of the frontal movement, including the timing of its arrival and speed of passage, is also of paramount importance, and this requires us to employ model domains sufficiently large to capture the front's parent storm system throughout the model simulation. This daunting combination is addressed with grid nesting. We used three nested domains having horizontal resolutions of 36, 12 and 4 km, respectively. The outermost grid crudely captures the entire storm system over the forecast period while the innermost domain concentrates the highest resolution in the local basin.

Two simulations were undertaken, both commencing at 4 PM local time on February 6th, approximately 24 hours prior to the onset of heavy rain. The lead-time gave the model a chance to “lock on” to the storm and guide it towards the LA area. The first, or control, simulation was started with observations valid at 4 PM local time but made no use of observations collected subsequent to 4 PM. The second of the two simulations employed a technique known as Four Dimensional Data Assimilation (4DVAR), a way of incorporating the subsequent observations into the model as it runs. The 4DVAR simulation represented an attempt to keep the model consistent with reality as it unfolded. Both simulations were integrated for 48 hours, fully spanning the time required for the storm to pass through Southern California.

Ideally, output from each simulation would have been compared to observed 48-hours precipitation accumulation over the basin collected at local range gauges. However, the gauges came in different types and styles, having different capacities and maintainers, and even incommensurable data collection intervals.

Further, the gauges were relatively few in number, not optimally distributed, and often not sited in the areas of greatest interest.

Figure 1 shows the topography of the Los Angeles region, while Figure 2 depicts the 48-hour precipitation accumulation in the control run's innermost domain, superimposed (black contours) on the local topography. The largest totals are found on the mountain slopes that happened to face the wind during the storm passage. The front passed from west to east, but in the hours prior to its passage, a strong southerly flow entered the LA basin. This flow pushed copious amounts of moisture up and over the basin's mountains from the south, producing rainfall that accounted for a significant fraction of the 48-hour total.

The locations of some of the rain gauges in the LA area are also superposed on Figure 2. Gauges too close to the boundaries of this domain have been excluded. It is worth noting that there are forty times more surface grid points than gauges in the innermost domain. Figure 3 shows a scatterplot of model predicted versus recorded rainfall for the control run. The predictions were made by interpolating the model output to the rain gauge sites; a task made more daunting by the rapid variation of elevation in the vicinity of some of the gauges (especially those receiving the most precipitation, since elevation is clearly a major contributing factor). While the overall trend seemed acceptable, the control run was judged to have produced excessive precipitation overall, especially on the mountain slopes that received the largest totals. Figure 4 shows that the 4DVAR run, in contrast, was found to under-predict precipitation at most locations, especially the interior basin locales at which the rainfall totals were relatively smaller. A comparison of the two simulations suggested that the 4DVAR technique resulted in a slower moving front with weaker southerly flow ahead.

Comparing the two simulations was made very difficult by the problem of having such a wealth of information. There were many gridpoints, prognostic variables, and time steps within an integration. In short, the two simulations were found broadly to differ, but how could those discrepancies be properly unpacked and presented? What, why and where did the two runs diverge? It was not a problem for simple summary statistics or histograms or statistical tests of these characterizations

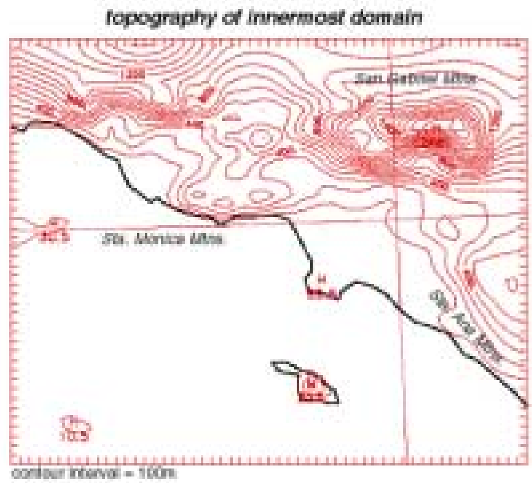


FIG. 1. *Topography of the MM5 model's innermost domain, centered on the Los Angeles basin. Contour interval is 100 m.*

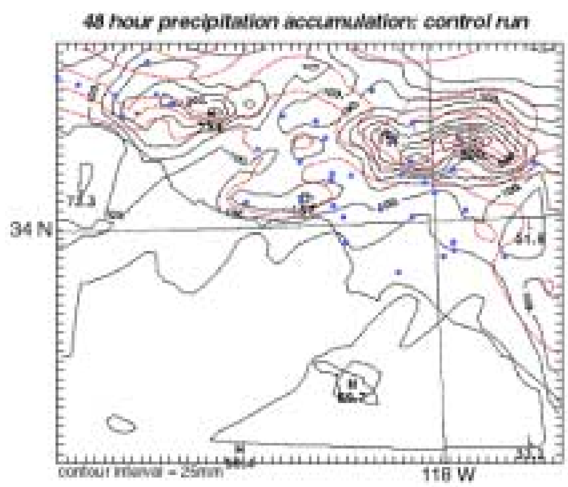


FIG. 2. *48 hour precipitation accumulation in the innermost domain for the control run. Contour interval is 25 mm. Dots mark the locations of rain gauges used in Fig. 3.*

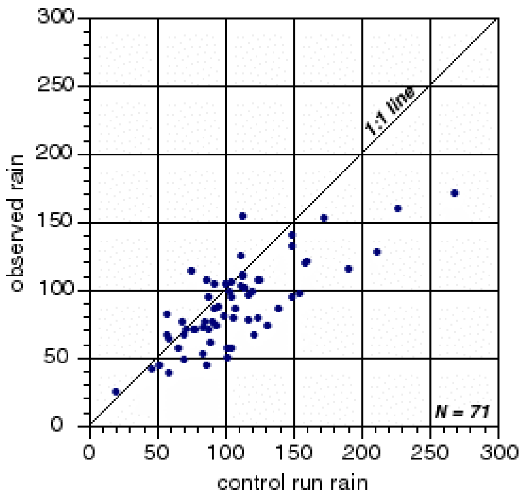


FIG. 3. *Scatterplot of observed versus predicted precipitation accumulation, using data from the control run. The 1:1 correspondence line is also shown.*

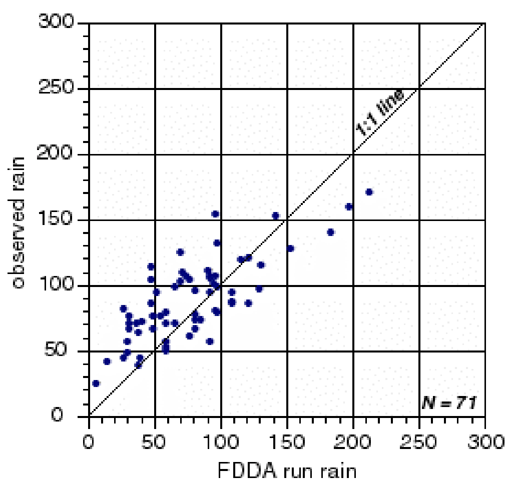


FIG. 4. *As in Fig. 3, but using the predictions from the 4DVAR simulation.*

In pointed contrast, the comparisons of model forecasts with reality were greatly hindered by the paucity of data. Precipitation, for example, is the end product of a huge number of interactions and processes, many occurring over time and space scales beyond the reach of our instruments. That made it more important to utilize what data there are, from whatever source, to find clues that may help identify the source(s) of forecast errors. This also was not a problem for simple summary statistics and conventional tests.

3.1.2 The Statistical Assessment
Presenter: Richard Berk, University of California at Los Angeles

In the simple terms, the problem to be solved was, how does one determine which of these two simulations is "right?" The answer, if any, should depend upon the particular context in which the simulation results were going to be used.

In this instance, the goal of the modeling was to provide precipitation information to hydrologists for their research. Thus, where the rain fell was as important as how much. Among other things, the hydrologists were interested in potential flooding. Heavy rain falling on one side of the Los Angeles coastal mountains would send the water into a different watershed than rain falling on the other side of the Los Angeles Coastal Mountains. For the hydrologists, a certain level of modeling precision was essential. Errors of several centimeters in total rainfall for a given storm, for instance, could be devastating. It might mean the difference between a serious flood and rainfall that could be contained within the existing storm water infrastructure. Moreover, ad hoc "fixes" for the modeling would be unacceptable. Since the hope was to use the model for the wide range of storms that can reach the Southern California coast, an ad hoc fix forcing a simulation to "fit" for one storm would not quarantee that it would "fit" for others. So it was essential to understand the causes of any modeling errors and to make structural changes in the model as necessary.

Given this context, there were a number of difficulties to be faced in evaluating the models. The existing data were sparse and collected from rain gauges that were not ideally located. For example, there were very few rain gauges at higher elevations, precisely where rainfall is likely to be the heaviest and most heterogeneous. There were initially few hunches about how the model outputs differed or why. Complicating matters was the common observation that there could be lots of things wrong with the models. There was initially no idea about which things were likely to be most wrong.

The strategy that followed was to see what could be learned from a comparison between the output from the two models and also between both sets of output to what "ground truth" data existed. In the interest of time, only the simulation comparisons were addressed at the workshop. Here the idea was to link significant disparities between the output from the two simulations to variables that might suggest what was going wrong (e.g., elevation). In so doing, we proceeded from very simple statistical summaries that disgard lots of information to more complex statistical summaries that discard less.

This exploratory data analysis perspective, trying to understand how and why the two outputs differed, is more appropriate in this context than confirmatory statistical inference (tests or confidence intervals). Both simulations had to be treated as effectively deterministic, so differences in output were also effectively deterministic. The computer models themselves were deterministic by design. To be sure, some data were used for initialization, but these data were not a probability sample of anything and were generated by essentially unknown procecesses. To represent formally the uncertainty implied would required the construction of a convenient fiction whose assumptions could not have been tested. We proceeded, therefore, conditioning on the data.

Similar issues arose with the data to be used for model evaluation. Certainly the data were stochastic, but the measured precipitation totals were both spatially and temporally dependent and came from a convenience sample of rain gauges. In addition, the nature of the measurement error was unknown. Consequently, we saw no way properly to map conventional statistical inference onto the problem at hand. Ritual statistical inference would have enlightened no one, even though statistical tests on deterministic models are de rigueur in some atmosphereic science circles (e.g., chapters 7 and 8 in von Storch and Narvarra, 1999.)

We began with the simple descriptive statistics. It was apparent that means differed enough to matter. In particular, the control run predicted more rain on the average, and the simple difference was large enough to matter in scientific and policy terms. Histograms of both sets of outputs revealed strong skewing to the right. Most of the predicted rainfall from the two simulations clustered at smaller rainfall amounts. But the 4DVAR run had many more observations piling up around zero.

A scatterplot constructed from the two sets of output showed a strong linear association and indeed, the correlation between them was 0.93.However, the fact that 4DVAR histogram showed more predicted rainfall amounts clustering near zero suggested that disparities between the two sets of outputs might have had an important spatial component.

Given the topography of the Los Angeles basin, longitude, latitude and elevation should be related to precipitation. We began, therefore, simply trying to summarize the conditional means of precipiation as a function of these three predictors. A simple linear regression was applied in which the arithmetic differences between two model outputs were regressed on those three variables. Overall, the results suggested that as one moves to the northeast and to higher altitudes, the simulations are more in agreement. As such, the results provided some initial clues about differences between the two simulations.

But the regression fit was poor and a wide range of regression diagnostics indicated that the specification was a least very incomplete. For example, sliced inverse regression clearly indicated that we needed far more than a 1D structure and that in fact, 3D structure would perhaps be required. One implication was that we needed to fit a surface that allowed for non-linearities and product variables.

The topography of the Los Angeles basin is in fact highly complex, and a complex response surface was implied. Moreover, an examination of the final response surface provided a number of insights. For example, the simulation output seemed to differ most as the storm hit the front edge of the coastalrange. More generally it now seemed clear that the disparities between the models had important scientific information, that the disparities had strong spatial relationships, and that these might be explained by differences between the two simulations in the angle at which the storm approached the coast.

What might be concluded from this exercise more generally about the role of statistics in computer model evaluations? Perhaps most important, there was a need to approach the virtual world produced by the models with the same care that one would employ for the real world. This implies the need for careful description as the foundation for understanding. In the eyes of many statisticians this exploratory data analysis is "blue-collar" work in which formal models to capture uncertainty are sorely missed. However, if formal models are applied without sufficient understanding of the virtual world being constructed, those models will be irrelevant or worse.

3.2 Wildfire Modeling

3.2.1 The Scientific Problem and the Model
Presenter: Rodman Linn, Los Alamos National Laboratory

In order to facilitate better decision-making about wildfire behavior, response, and effect, researchers have been working to model wildfires for more than a half century. These relevant decisions can include long term and short term components. In the long term, for example, wildfire models can be used to better understand various fire prevention strategies, such as controlled burns. In the very short run, wildfire models can be used to help direct in real time the responses to a particular wildfire, such as where to place fire fighters and when to move them.

The majority of the operational wildfire models currently in use are empirical and have been developed based on a limited number of idealized experiments. Because of the limited number of wildfire types used to develop these empirical models, they are not appropriate in many wildfire circumstances. These empirical models are also limited in their ability to model the strong coupling among the many physical processes that exist in a wildfire (heat transfer, chemical reactions, moisture extinction, buoyancy induced turbulent flows, flow through canopy, etc.), and are thus limited in their ability to predict emissions and ecological effects of wildfires.

LANL is developing a wildfire model, FIRETEC (1), which is based on simulating the physical processes that control wildfire behavior. FIRETEC captures the combined effects of small micro-events on the macro-scale fire behavior. It can be used to model fires and their effects in most realistic wildfire circumstances (complex terrain, variable wind conditions, nonhomogeneous vegetation), including those that are impossible to simulate accurately with current operational models. The principles of conservation of mass, species, momentum, and energy are the basis of FIRETEC. Customers for this model include land managers and firefighters. To view graphical output from FIRETEC see https://wwwproxy0.lanl.gov/AUTO/http://www.lanl.gov:80/delphi/projects/wildfire-rams.shtml.

Coupled transport equations are the mathematical framework for FIRETEC. These transport equations (written in the form of partial differential equations) incorporate time and space history into expressions for momentum, internal energy, gaseous species concentrations, turbulent kinetic energy, and fuel moisture depletion. An example of one of these transport equations is given in symbolic form in Equation 1. Equation 1 describes the transport equation for internal energy for the combined gas phase in the presence of a wildfire.

$$\begin{aligned} \frac{\partial(Internal\ \ Energy)_{gas}}{\partial t} = \ & (mean\ \ flow\ \ advection) \\ & + (Diffusion\ due\ to\ turbulence) \\ & + (Net\ radiation\ source\ to\ gas) \\ & + (Net\ convective\ heat\ exchange\ to\ gas) \\ & + (\ Internal\ energy\ source \\ & \qquad due\ to\ chemical\ reactions) \end{aligned} \tag{1}$$

The various terms depicted on the right side of equation 1 are strongly coupled with terms in other transport equations as shown in the following table

Term in Internal Energy Equation	**Other transport equations that this term is directly coupled to**
Mean flow advection (average rate of horizontal flow of gas)	Equations for Momentum
Diffusion due to turbulence	Turbulent kinetic energy equation
Net radiation source to gas	Gaseous species concentration equations Internal energy of the solid fuels
Net convective heat exchange to gas	Internal energy of the solid fuels Equations for Momentum 3 directions
Internal energy source due to chemical reactions	Turbulent kinetic energy equations Gaseous species concentration equations Internal energy of the solid fuels

This coupling makes it very difficult to isolate and evaluate specific processes that are occurring in a wildfire. The coupling also makes it very easy for a small error in models of a single process or quantity to propagate to the representations of other processes or quantities. Inaccuracies in input data are also prone to have very complex ramifications in such a complex model, and the outcome of such a model will often be altered in unforeseen ways. Therefore, a systematic statistical uncertainty analysis is critical for understanding the uncertainties of this type of physics-based model, and for understanding how sensitive the results are to inaccuracies in input data.

Physics-based wildfire models have the ability to predict very detailed behaviors such as individual wind gusts, specific details of fire-line shape, and locations where vegetation is not completely burned. The presence and nature of some of these fire-behavior details helps give the models like FIRETEC credibility because qualitatively similar features occur in nature. However, the specific location where there is a patch of fuel that is not burned, the specific point on a fire-line that sticks out ahead of its neighbors, or the moment that a gust erupts from a fire are all details that are very dependent on unresolvable input details (the specific vegetation configuration, the small in coming wind gusts, etc.) These unresolvable input details are not measured accurately but have large effects on precise nature, location, and timing of some on the fire-behavior details.

To further complicate matters, it is very difficult obtain actual wildfire data for model evaluation. The difficulty in obtaining these data results from the difficulty of getting adequate comprehensive instrumentation deployed on a true wildfire. Currently data from controlled burns are used to evaluate the wildfire models. However, there are a limited number of conditions under which the controlled burn experiments may be performed. These experiments help to validate particular aspects of wildfire models, but do not allow evaluation of the overall wildfire model under a variety of conditions.

3.2.2 The Statistical Assessment
Presenter Frederic Schoenberg, University of California at Los Angeles

FIRETEC presents particularly difficult problems for model evaluation and as such may represent well a worst case scenario for statistical tools. There are perhaps two broad types of model evaluation: internal and external. Internal model assessment is the evaluation of the structural relationships prescribed by the model. For instance, a model for the spread of wildfires may be based on relationships between spread rate and variables such as wind, temperature, vegetation, fuel moisture, precipitation, and so on. Some of these relationships could be examined individually. Such internal model evaluation is most often done using laboratory experiments, where each of the variables can be carefully controlled and measured. Unfortunately, the relevance of such evaluations can be questionable because of scaling problems. For example, most experiments on fire behavior involve fires of sizes on the order of inches; extrapolation of such results to multi-acre forest fires could be spurious.

Alternatively, one might examine the external features of the model: how well the model describes the broad features of the phenomenon in question. For instance, one can observe actual forest fires and see if their behavior in certain aspects of interest – e.g. temperature, burn pattern, flame angle, and spread rate – agree with the model. Unfortunately, obtaining the appropriate model input data to generate model output for such comparisons is very difficult.

One approach to this problem might be to use a statistically equivalent model (SEM) to help identify the input space that produces the real world observations. The SEM is used as what Brieman (2001) calls an algorithmic model. That is, the goal is to link inputs to model outputs without trying to explicitly represent the underlying causal mechanisms. The compter model is treated as a black box. Such an approximation can be useful for various purposes including the description, inversion, and simulation of the model. The coefficients of a SEM might be more easily interpreted and thus could highlight important features of the computer model. Further, while the complex FIRETEC model is costly to run and difficult to invert, such might not be the case for a SEM.

One specific SEM technique, which could be useful is to approximate FIRETEC by a locally linear, space/time-invariant filter (Schoenberg et al., 2000.) By locally linear, we mean that the output perturbation resulting from a perturbed input is a linear function of the input perturbation. By space/time invariant, we mean that the relationship between perturbed inputs and outputs does not vary with location and time. The idea is that FIRETEC, though perhaps highly nonlinear, may be locally nearly linear. The benefit of approximating FIRETEC in this way is that local linear systems are very easy to simulate, invert, and interpret. This suggestion was interesting to the FIRETEC modeler, but had not been attempted at the time of the workshop.

3.3 Transportation Modeling – Design and Evaluation of Traffic Signal Timing Plans

3.3.1 The Scientific Problem and Model
Presenter: Nagui Rouphail, North Carolina State University

The development of efficient signal timing plans for urban traffic networks is a continuing challenge to traffic analysts and engineers. Flows on these networks, even small sub-networks, are highly complex: they encompass a variety of vehicles (autos, trucks, buses), pedestrian-vehicle interactions, driver behavior, and an assortment of network conditions (lane arrangements, stop signs, parking lots, one-way streets). Moreover, the traffic demands on the network are highly variable (minute-to-minute, hour-to-hour, day-to-day, month-to-month) as are many of the movements (even legal ones) of vehicles and pedestrians.

Over time and through experience and modification traffic managers have developed signal control strategies to respond to these conditions. In recent years they have been assisted by traffic models, sometimes oversimplified, that can generate signal control strategies (see Click and Rouphail, 1999, for a review of a number of these).

At the same time, there has been a steady development of microsimulation computer models that simulate traffic under a complexity of conditions, including traffic signal settings. One such, Corridor Simulation (CORSIM) has been adopted by the Federal Highway Administration (FHWA) as the quasi-official platform upon which to gauge traffic behavior and compare competing strategies for signal control before implementing in the field. This leads to two crucial questions: first, how well does CORSIM reproduce field conditions and second, can CORSIM be trusted to represent reality under new, untried conditions (e.g., revised signal timing plans)?

To address these questions we undertook a case study, with the cooperation of the Chicago Department of Transportation (CDOT), and the Urban Transportation Center (UTC) of the University of Illinois at Chicago. The test-bed for the study is the network depicted in Figure 5. The case study involved data collection for inputs required to run CORSIM as well as data to evaluate CORSIM's capability to model field conditions. Performance measures were defined on CORSIM output and were used to determine optimal signal parameters.

CORSIM is a stochastic simulator that moves vehicles second by second through a network. Three types of inputs are required:

1. Fixed and non-controllable inputs: The network in Figure 5 represents a set of urban streets within the City of Chicago. In CORSIM, streets and intersections are modeled as directed links and nodes, respectively. Specification of the network includes a set of fixed inputs describing the geometry (e.g., distance between intersections, number of traffic lanes, length of turn pockets), the placement of stop signs, bus stops and routes, and parking conditions.

2. Random and non-controllable inputs: Vehicles – autos, trucks, and buses – are generated by sampling interarrival time distributions at each entry node of the network. The interarrival time distributions are assumed to be independent (vehicle-to-vehicle, node-to-node), and may be different for each entry node. The designation of vehicle type – auto or truck – is made through independent Bernoulli trials with a fixed probability estimated. from field data. Buses are treated according to their schedule and routes, with random dwell times at bus stops and random interarrival times at entry

nodes. The behavior of the traffic is affected by additional random factors such as turn probabilities, driver characteristics (car-following behavior, lane changing r… provided in the CORSIM softwa… aggressiveness) while others (suc… d or specified.

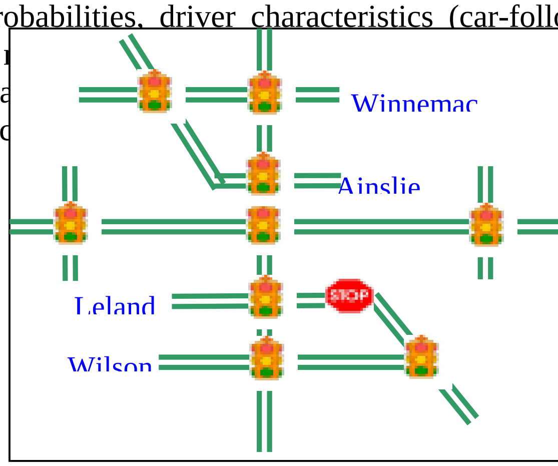


Fig 5. Test-bed network.

3. Controllable inputs: For a signal study, the signal settings must also be specified:

    - *cycle length* – we assume a common cycle length for all signals
    - *green times* at each intersection – how long the signal is green for straight through movement, protected left turns,
    - *offsets* – the difference in time between the start of the "green" through-movement at a signal and the time of the start of the green through-movement at a reference signal.

For the network of Figure 5 there are 22 signal parameters: 1 cycle, 13 green times, 8 offsets.

One hour of traffic, about 7500 vehicles total, takes about 1 minute to simulate on a PC with a Pentium II-500 Mhz. The status of each vehicle is updated every second. While each run is fairly quick, the need for many runs to deal with the substantial variability induced by the stochastic assumptions and the optimization of the signal parameters makes the time for an experiment non-trivial. Each experiment required 625 runs, taking approximately ten hours per experiment.

CORSIM comes equipped with an animation package that enables visualization of the traffic movements, a capability of great value in exploring the characteristics of the model and detecting problems and flaws. Besides the visual output, CORSIM provides aggregated (over selected time intervals such as the signal cycle) numerical output for each link: number of trips on each link, average link travel time, link queue time (the sum over vehicles of the time, in minutes, during which the vehicle is stationary, or nearly so), maximum queue length on each lane in the link, link delays (simulated travel time minus free-flow travel time, summed over all vehicles traversing the link). It is from these outputs that performance measures are taken.

3.3.2 The Statistical Assessment
Presenters: Jerome Sacks and Byungkyu Park, National Institute of Statistical Sciences

The data available for this case study were collected during mid-week morning and evening peak periods, one hour each. A platoon of human “counters” was employed to count vehicle arrivals (cars, trucks) at each boundary (entry) node for the entire one-hour period in the morning and evening. Turning movements at all links were counted: some links for short periods (15 minutes), some for one hour. Total vehicle flows and maximum queue lengths were counted on key internal links over the one-hour periods.

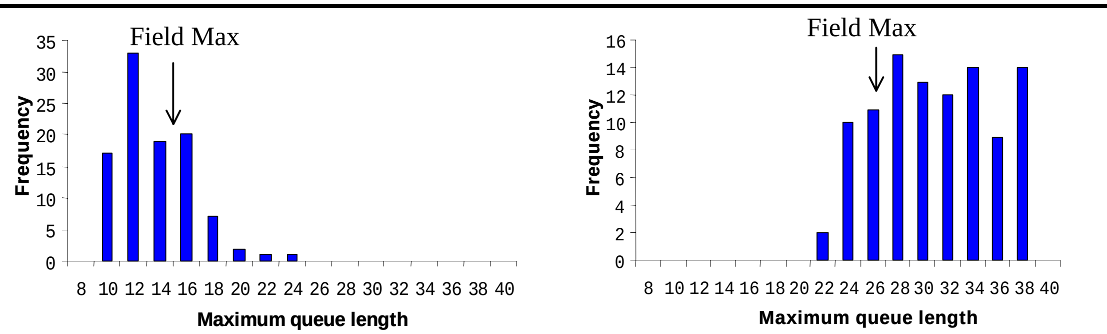
Input parameters were estimated from data as follows. The vehicle mix was estimated by observed proportion, as were the turning probabilities. The parameter of the interarrival time distribution at an entry node was estimated by a simple moment estimator of a parameter of a gamma distribution.

Using the estimated input parameters and the existing (base) signal plan we made 100 independent runs of CORSIM and viewed histograms of maximum queue length (MQL) for 6 key links (2 are plotted in Figure 6). This was done for the morning and evening periods. The observed field values are clearly well within the simulated ranges (as they were for the key links not shown in Figure 6) and tempts us to accept CORSIM traffic as a good representation of reality. But this would be highly heuristic and subjective. Traffic is inherently variable, but the variability reflected in the histograms in Figure 6 may be excessive. The dependence between MQL and the data used to estimate the inputs to the simulator is not accounted for, nor are the dependencies among the MQL histograms for the various links.

Explicit in the above process is the selection of an evaluation function, the MQL. There are many potential candidate functions that could be considered, and the selection is somewhat arbitrary, but motivated by two considerations: (1) the feasibility of collecting the corresponding field data and (2) the connection between large MQL and potential for spillback and gridlock (nightmare conditions for traffic managers). (Spill back occurs when congestion causes traffic to back up and block movement at an upstream interesection. Failure of Spillback to clear up can result in gridlock.)

Because spillback and gridlock were not observed in the field, the presence of either in several of the repeated simulation runs can be a sign of problems with the simulator. That presence may be numerically indicated by low throughput (number of completed trips) and by large “run-to-run” variance. For example, an optimal signal strategy (call it SS1) produced, in 100 runs, a mean queue time of 224.3 hours, a median of 180.9, and a standard deviation of 90.8 hours.

This high variability led to a close examination of the animation to uncover the circumstances leading to such large queue times. This in turn led to the snapshots (the 17:36:25 animation snapshot and the 17:23:30 one) in Figure 7, which show the formation of spillback and gridlock. The cause was found to lie in the presence of a stop sign (at the upper right part of Figure 7) with overly long stop times. These are not found in the field because of the common practice of "rolling stops", at least when police cars are absent. Indeed, when the stop sign was altered to reflect this reality the results were striking: the optimum plan under the new circumstances had mean queue time of 122.5, median 111.2, a standard deviation of 34.4, and an absence of spillback.



(a) Southbound (100 CORSIM simulations) (b) Northbound (100 CORSIM simulations)

FIG 6. *MQL distribution from CORSIM and field at intersection of Western and Lawrence (see Fig. 5).*

(a) Snapshot taken at 17:36:25 (b) Snapshot taken at 17:23:30

FIG. 7. ANIMATION SNAPSHOTS FROM AN OPTIMAL SIGNAL STRATEGY (SS1)

To find optimum signal plans we adopted an objective function that minimizes a modified network queue time (MNQT):

$$MNQT = \sum_{i=1}^{L}\left[QT(i)\times\left\{\max\left(1,\frac{MQL(i)}{SC(i)}\right)\right\}\right]$$

where: *QT(i)* = queue time on link I, I= 1,2,…., L
MQL(i) = maximum queue length on link I
SC(i) = through signal capacity on link I, a function of the cycle and green time on link i.

Thus, we seek to minimize the network-wide queue time while penalizing overly long queues. The penalty avoids solutions that reduce queue time on a busy link at the expense of long queues on a less busy link. Optimizing this function over the 22 signal parameters was done via a genetic algorithm (Goldberg, 1989) applied to this stochastic optimization problem where the objective function is observed with error – the observation being a result of a single CORSIM run. An earlier effort via response surface fitting could not cope with the high degree of dependence among the offset parameters, the substantial run-to-run variability in the simulator, nor the non-smooth dependence of the objective function on the offsets. Having found an optimum this way, an additional 100 runs were made to compare the distribution of queue time of the optimum plan with other plans, especially the (current) base plan. These plots are shown in Figure 8.

To treat the uncertainties generated by the input data and the dual-use of the collected data for model inputs as well as for evaluation, we will need a more elaborate framework, possibly utilizing ideas from Bayarri and Berger (1999).

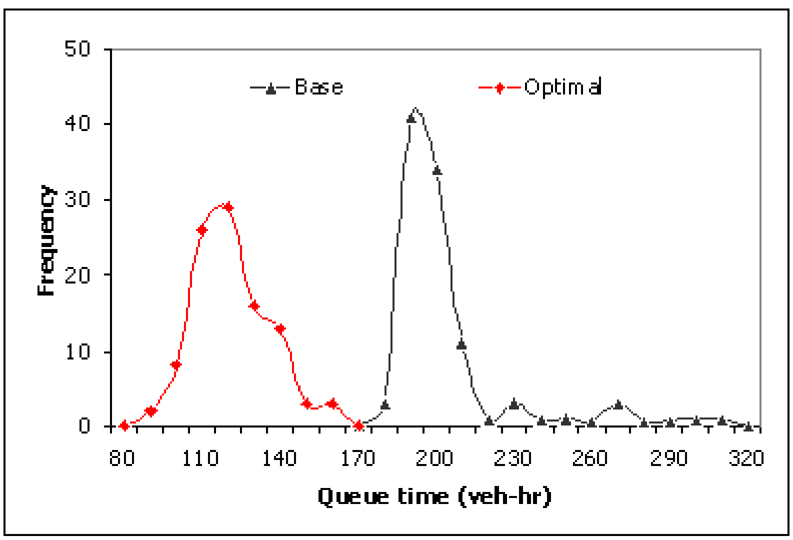


FIG. 8. *Queue time comparison between optimal and base case*

Lessons learned from the case study include:

a) designing and collecting field data is critical, difficult, and expensive,

b) robustness in the "simulator" world is not necessarily robustness in reality. It would be poor advice to just tell the Traffic Commissioner to change signal plans without an accompanying caution that a follow-up study is necessary,

c) the use of visualization (in CORSIM, the animation) is important because it can quickly provide insight into difficulties and also assist in uncovering sources of trouble.

3.4 Influenza Modeling – Annual Influenza Vaccination

3.4.1 The Scientific Problem and the Model
Presenter: Alan Perelson, Los Alamos National Laboratory

In a typical flu season between twenty and forty thousand people die from the complications of influenza infection. Vaccination is our major weapon in protecting against flu, and each year tens of thousands of people get vaccinated. In the 1970's and 1980's two large clinical studies addressed the question of whether people vaccinated one or more times in the past were better protected than people getting a flu shot for the first time (Perelson 1979, Keitel et al 1997, Smith et al 1999,). Surprisingly, they reported conflicting results: in some years it appeared that first-time vaccinees had better protection than repeat vaccinees, while in other years the reverse was the case. In a recent study, Smith et al (2000) proposed a computer model that embodied in a schematic way a plausible qualitative feature of the immune system referred to as the antigenic distance hypothesis. The researchers used this model to explain the heterogeneity of repeated annual influenza vaccination. The antigenic distance hypothesis is illustrated in Figure 9.

The computer model simulates the antibody response to influenza vaccination and to exposure to an epidemic strain of flu virus. The model is agent based and considers a population of 10^7 B lymphocytes, the cells that secrete antibodies. In the model each B cell is characterized by having a randomly made receptor specified by a string of 20 characters on a 4 letter alphabet. This formal characterization suffices to capture the complexity needed for this process, It does not have a physical interpretation. Distances represented in two dimensions in Figure 9 are actually Hamming distances in 20-dimensional space in the model. (Hamming distance is a measure of the difference between two finite strings of characters, expressed by the number of characters that need to be changed to obtain one from the other.) When a B cell is stimulated it secretes its receptor as a soluble molecule called antibody. In the model, flu viruses are also characterized by a similar length string and Hamming distance is used to compute the "antigenic

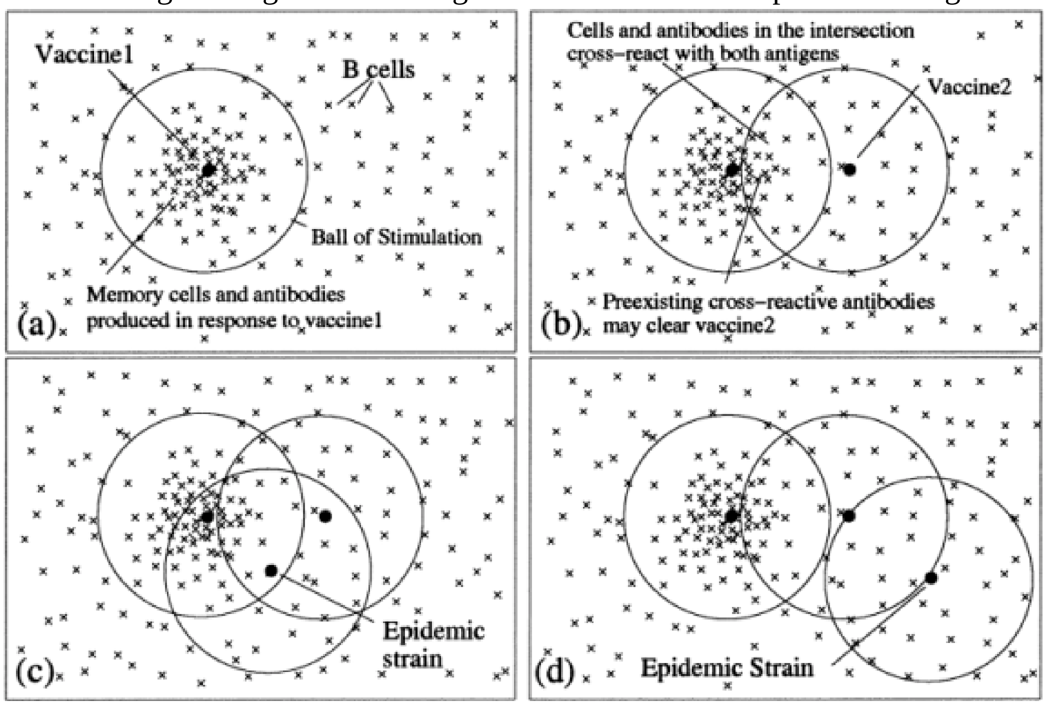


FIG. 9. *An illustration of the antigenic distance hypothesis. The affinity between a B cell or antibody (×) and an antigen (solid circles) is represented by the distance between them. (In the figure the plane is used as an inadequate representation of string space (20 dimensional space endowed with Hamming distance.) Similarly, the distance between antigens is a measure of how similar they are antigenically. (a) B cells with sufficient affinity to be stimulated by an antigen lie within a ball of stimulation centered on the antigen. Thus, a first vaccine (Vaccine1) creates a population of memory B cells and antibodies within its ball of stimulation. (b) Cross-reactive antigens have intersecting balls of stimulation, and antibodies and B cells in the intersection of their balls. Those with affinity for both antigens are the cross-reactive antibodies and B cells. The antigen in a second vaccine (Vaccine2) will be partially eliminated by preexisting cross-reactive antibodies (depending on the amount of antibody in the intersection), and thus the immune response to Vaccine2 will be reduced (8, 9). (c) If a subsequent epidemic strain is close to Vaccine1, it will be cleared by preexisting antibodies. (d) However, if there is no intersection between Vaccine1 and the epidemic strain, there will be few preexisting cross-reactive antibodies to clear the epidemic strain quickly, despite two vaccinations. Note that in the absence of Vaccine1, Vaccine2 would have produced a memory population and antibodies that would have been protective against both the epidemic strains in c and d.*

distance" between a virus and antibody or B cell. How well a flu virus matches the receptor on a B cell (e.g. how well virus proteins fit into receptors), is represented in the model by a the antigenic distance, which ranges from 0 to 7. Zero is a perfect match. If there is a partial match, we assume the virus antigen can stimulate the B cell into reproduction and further antibody production.

Antibodies that are partially matched to a flu virus (the antigen) bind the flu virus and lead to its elimination. Binding is viewed as a stochastic phenomena. For example an antibody has a certain probability of binding the virus depending on antigenic distance and other paramters, which are specified. The probabilistic representation of binding for both antibody generation and removal of antigens provides the stochasticity to the model.

The computer experiment considered two influenza seasons, one year apart, with four categories of individuals: (*i*) those never vaccinated, (*ii*) those who received "Vaccine1" (v1) at the start of the first influenza season and were not vaccinated for the second season, (*iii*) those not vaccinated for the first season but who received "Vaccine2" (v2) at the start of the second season ("first-time vaccinees"), and (*iv*) those who received v1 at the start of the first season and v2 at the start of the second ("repeat vaccines"). All simulated individuals were challenged with epidemic virus two months into the second influenza season. The same v2 and epidemic strains were used for all simulated individuals, and v1 was varied. The antigenic distance between v2 and the epidemic (v2-e distance) was fixed at 2. Since cross-reactive distances vary between 0 and 7, this distance is "close," but it is not a perfect match. The v1-e and v1-v2 distances varied between 0 and 7. The vaccine strains were nonreplicating, whereas the epidemic strain was able to reproduce. During each simulation if the viral load exceeded a "disease threshold" the simulated individual was considered symptomatic. Each experimental group contained 200 simulated individuals, and the attack rate within a group was defined as the proportion of the group in which the viral load exceeded the disease threshold. The results of the experiments, reproduced from (5), are shown in Table 4. A simulated individuals vaccine, "real antigens," antibodies and T-cells were randomly generated according to rules based on antigenic distance and other parameters. Details are provided in Smith et al (2000).

Table 4
Summary of experimental attack rates

v1-e		v1-v2 distance for repeat vacinees							
distance	v1 only	0	1	2	3	4	5	6	7
0	0.01**			0.00**					
1	0.46		0.06**	0.01**	0.04**				
2	0.87#	0.78#	0.37**	0.20**	0.19**	0.18**			
3	0.96#		0.74#	0.44*	0.36**	0.35**	0.38**		
4	0.99#			0.71#	0.50	0.45*	0.41**	0.50	
5	1.00#				0.66¶	0.46	0.47	0.50	0.50
6	1.00#					0.65¶	0.54	0.45*	0.54

7	1.00#		0.55	0.58	0.52

The fraction of individuals who develop flu symptoms, i.e., the attack rate, in the unvaccinated control was 1.0 (not shown). The attack rate for first-time vaccines (v2-only) was 0.55 (not shown). Attack rates for repeat vaccines and the v1-only groups are shown in the table. Groups marked with a ¶ or # had higher ($P < 0.05$ or $P < 0.01$, respectively) and groups marked with an * or ** had lower ($P < 0.05$ or $P < 0.01$, respectively) attack rates than did first-time vaccines. Attack rates as high as 1.0 are due the large-dose experimental challenge of each simulated individual.

One immediate conclusion from the table is that repeat vaccination is always beneficial when given to previous vaccinees. This is illustrated in that the attack rates in each row are lower for the repeat vaccinees than for the individuals who received vaccine 1 alone. We also compared the simulation results to the two clinical trials that have evaluated the benefits of repeated annual vaccination, using data supplied by the Centers for Disease Control and Prevention, Atlanta, to estimate the antigenic distances between the various vaccines and epidemic strains in the study years. Figure 10 shows that the computer simulations had surprising agreement with the experimental observations.

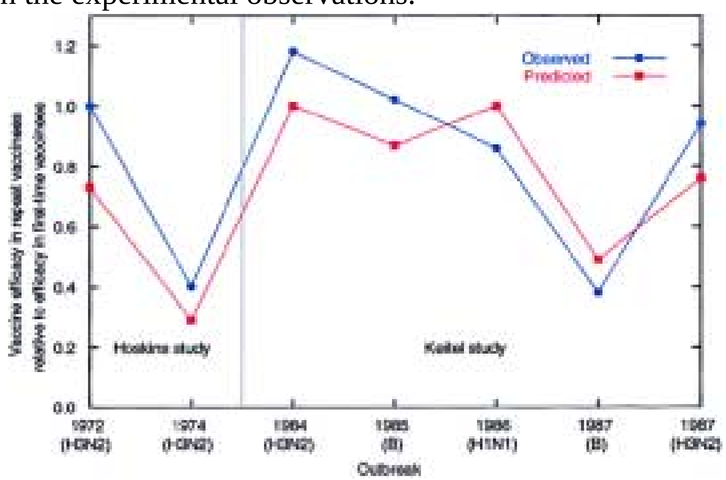


Fig. 10. Observed vaccine efficacy in repeat vaccines relative to the efficacy in first-time vaccines, and predicted vaccine efficacy based on the antigenic distance hypothesis.

1.4.2 The Statistical Assessment
Presenter: Peter Bickel, University of California Berkeley

Immune system modeling raises most of the issues addressed in this workshop. The goals are on the one hand purely scientific, understanding how the second most complex system of the body works, and on the other hand very practical using models to predict the effect of vaccines and the progression of diseases such as HIV. The antigenic distance model is particularly inviting to statisticians since it is purely stochastic. All objects, various types of B cells, antigens, antibodies are modeled as bit strings, their interactions and life histories are purely stochastic. The antigenic distance model can be thought of as a continuous time, finite state Markov process, each of whose states is an array labeled by the 20 possible bit strings and the 400 pairs of bit strings. Corresponding to each bit string is a vector of counts recording how many unbound antibodies, antigens, memory and plasma B cells etc., corresponding to that bit string are present at that time. Corresponding to each pair of bit strings is the number of bound antigen-antibody pairs. Events such as binding, birth and death of cells occur with exponential lifetimes determined by the current state of the system and then change the current state according to a transfer matrix e.g., binding of an antibody with an antigen reduces the corresponding count entries at their two bit strings by one and adds to the count of bound antigen-antibody pair at the corresponding pair of bit strings.

Model Evaluation. Verifying whether such models represent the detailed working of the immune system is difficult because the detailed data come from small animal experiments. This may change as other richer sources of information such as gene array data come on line. On the other hand seeing how well such a schematic computer model fits and explains apparent anomalies in epidemiological data is, as shown above, very feasible, and the measures of performance are clear. For instance, given such a model, can one design vaccines with behavior predictable for given flu epidemics, at least *ex post facto*, knowing the type of the antigen causing this year's epidemic as opposed to previous years'?

Given predetermined intrinsic parameters, each run of the computer model produces attack rate data for set values of the three external parameters. What one is interested in is the behavior of the average attack rate over runs produced by the computer model as a function of vaccine-vaccine and vaccine-antigen distances, as well as the differences between model and observed (in epidemics) attack rates. All quantities observed have stochastic variability resulting from random seed differences in the model and in comparisons with real data unknown factors in the observations. Since one wants to make statements about all these parameters simultaneous inference is required. For studying the variability of the average attack rates over runs for fixed distance settings presumably the Gaussian approximation can be used. For studying the variability of average attack rates for different distance values variants of the Tukey or Scheffe methods (Miller, 1966) based on parametric bootstrap ideas (Efron and Tibshirani, 1993) are appropriate.

Computer Experiments / Computational Issues.For finding optimum vaccine regimes as a function of previously observed antigens and vaccine-antigen interactions, we need to maximize functions of combinations of distance settings, which are estimated from the averages over runs of outputs of the computer model. Such optimizations raise issues of sequential experimental design. For what combinations of distance settings should runs initially be made? How does one move to optimally search for the maximum? How many runs should be made at values of the parameter for which we count to estimate the function we are optimizing? This can depend on the model parameter values, etc. Methods for doing this have been considered in the statistical and engineering literature: see Box and Draper [1987], Kiefer and Wolfowitz [1952], and Kushner and Lin [1997] for surveys.

Stochastic cellular automaton models of the type considered above can be approximated by simpler stochastic models that might run more quickly. Evidently, implementation of the cellular automaton model does not follow the description given above; one would not wish to keep track of what happens at all bit strings or pairs of bit strings since most count vectors are 0's. In fact, given the definitions of affinities, one only needs to keep track of what is happening at various vaccine-antibody, vaccine-antigen distances. However, it would appear that a good deal of the time for implementation of the model comes from bookkeeping.

A coarser model might lump bit strings at a grid of vaccine-antibody, vaccine-antigen distances together and discretize time so that event rates are kept constant over fixed stretches. Then the discretized process is no longer Markov but hidden Markov. To generate it correctly one would in fact have to go to the original computer model and simply record less. However, if the lumping of states and discretization of time is not too extreme one might hope to approximate the generation of events by a Poisson vector with parameters depending on the state as described in coarsened form at the previous discretized time point. The transfer matrix would then combine the Poisson vector and previous state to give the current state

4.0 SUMMARY OF DISCUSSIONS

Following each session there was a lively open discussion led by a moderator and summarized by a rapporteur. These intent of these discussions was to answer the four questions described in the introduction in the context of the particular model. However, the discussions generally posed more issues than answers. Nevertheless, they were immensely valuable. The discussions stimulated thinking, raised awareness, inspired collaborations, and helped identify directions for future research. The following provides a summary of these discussions and the rapporteurs' syntheses of the discussions framed by the four questions. While this section captures some of the content of the discussions, it does not adequately convey their energy or enthusiasm. The following summary is compiled from notes, rapporteur vu graphs, tapes and reviewer comments; as such it does not necessarily reflect the opinions of the authors.

4.1 What do we mean by model evaluation?

This question met with the resounding response that to determine how good a computer model is, one must first answer the question "good for what?" Indeed, a clear message from the workshop was that there is really no such thing as a context-free model evaluation. A second message was that, while context is key, it is too often not taken seriously. A client's challenge, such as "what is this model good for?" may be required before the modeler begins to appreciate the ways in which context might matter.

During the discussions, components of context were identified including:

- Application. Applications include science, where the aims of the model are exploration and explanation; decision–making, where planning and policy are emphasized; and training, where the computer model simulates real world situations to which individuals respond.
- Consequence. Consequence refers to the real-world impact of the modeling, such as impacts on public health, traffic, flood control, or safety as described in the examples in Section 3.
- Accuracy. Accuracy refers to the precision needed for the task at hand. It is one thing, for instance, to qualitatively represent the gross behavior of a wildfire and quite another to use that model to tell fire fighters when to abandon a position.

None of the workshop examples included a training application (although one of the future goals of the wildfire control model was to be able to use it to help train fire fighters), but all have science and decision-making contexts. The application context for Mesoscale Model Version 5 (MM5) in the workshop example was to provide input to a hydrological model to predict streamflow and runoff in support of decision-making to mitigate flood disasters. The evaluation function was defined in terms of predicting spatially distributed 48-hour precipitation accumulation, the input to the hydrology model. What needed to be weighed were the consequences of error for not acting to prevent flooding when necessary, versus taking (costly) actions when not necessary. The probability of decision errors had to be small, thus requiring great accuracy for the input to the hydrology models. Output from two simulations of MM5 (in principle, two different models, one using Four Dimensional Data Assimilation (4DVAR)), were compared with data from a single storm event. Neither simulation produced the requisite accuracy. However, comparison of the two simulations revealed important differences between them, illuminating the science even though the decision requirements could not be met.

The immediate goal of the wildfire model FIRETEC was to facilitate better decision-making. A future goal was for the model to help guide the actions of fire fighters in real time (e.g., "evacuate an area now"). The consequences of modeling would then be serious indeed. Interestingly, the modelers aspired to these ambitious decision-making goals even though there was apparently no hope of capturing the exact behavior of any single fire.

The traffic model, CORSIM, was used both for scientific exploration (what factors are important when designing traffic signal timing plans?) and ultimately to support decision-making (which of a number of possible signal control strategies should be implemented?) The consequences of errors for the decision-making application ranged from irate phone calls to the traffic chief to major traffic congestion. An interesting result of the model evaluation was that when the model failed (unreasonably long queue times and unrealistic spillback), the failure led to insights about traffic modeling: rolling stops rather than complete stops are needed to capture driving behavior. This result supported the point made several times during the workshop that an incorrect model can still be useful. Moreover, it was noted in the discussion that one might be able to make a good decision, even if one could not make an accurate prediction.[3]

The influenza model application context ranged from the scientific concern of "does the model explain the phenomenon" to the policy concern of "should an individual be vaccinated each year?" The discussion raised again the prospect of gaining scientific understanding and/or making useful predictions even with models of the "emergent" or "phenomenological" type (in the terminology of Section 2).

4.2 What makes model evaluation difficult?

For this question there was no shortage of answers. One answer, common to all of the models, was "the available data are inadequate." Either the data were poor or limited. The rain gauge data for the storm model were poorly positioned and crudely measured. Data from wind tunnel experiments or controlled burns instead of real fires were the only data available for the wildfire model evaluation. These

[3] Subsequent to the workshop, a follow-up study was done on a larger, more complex network near downtown Chicago. Data were collected in May 2000 and a validation exercise similar to the one discussed in 3.3 was carried out. Flaws in the model were detected and adjusted for in devising a new signal plan and the recommended plan was implemented by the Chicago Department of Transportation in September 2000. Data were collected that confirmed the prediction that the new signal plan would improve traffic flow ("predictive validity").

data do not adequately represent the conditions of the uncontrolled wildfires. Data collection for the traffic model case study was costly and the data had serious quality issues. Data of sufficient detail to directly evaluate the influenza model could not be obtained. Instead detailed data from animal studies must be used in the simulation and high-level model predictions compared to limited real-life human data.

It appeared to some that model evaluation produced a difficult double-bind. Models are necessary to predict/understand phenomena when there are very limited or no data. But without data, model evaluation is extremely difficult. So, when you need models the most, they are least likely to be reliable. In addition, the statisticians in the audience (and perhaps others) felt that the modelers did not sufficiently emphasize or plan for the collection of data on which model evaluation might be based. There was also concern that modelers were not aware of, or at least had not considered using, rich new sources of data. A few participants even wondered if in some instances the modelers were ignoring the data that might answer the scientific or policy question better than any of the existing computer simulations.

At the same time, for many applications raw data as such does not really exist. It comes having already been massaged by various physical devices, computer algorithms, and statistical computations. Thus a comparison between simulation output and data, for example, is really a comparison of two amalgamations differing in the amount and use of external information. Moreover, the data are often not observations of the physical variables needed for comparison with the model. In these cases, there is a secondary model that takes the raw data and converts it to the quantities that will be used in the model evaluation. In short, the data used in model evaluation are far from pristine and this adds another layer of uncertainty and difficulty to the model evaluation process.

Other issues identified as making model evaluation difficult included the following:

- *Qualitative comparisons.* There are qualitative measures as well as quantitative measures for model evaluation. In some cases, what most interests a modeler may be emergent qualitative behaviors, such as traffic jams or agreement with epidemic data.

- *Data / model dependencies.*

  <u>Data assimilation</u> is difficult and takes many forms, some of which do not have sound statistical foundations. The criteria used to evaluate a model with ongoing data assimilation may be different from those for a model used to make forecasts without such information. Indeed, it may make little sense to use the same data for model corrections and later, model evaluations.

Calibration is difficult given the large number of variables involved. If calibration has to be done on the same data used for validation (as is often the case in statistics), then the evaluation becomes model dependent and less credible (unless account is taken of the dual use).

- *Propagating uncertainties.* There are diverse, numerous, and poorly understood sources of uncertainty: in the science, the translation of the science into computer code, and in the numerics, software bugs and hardware, as well as data.
- *Computational requirements*. The size, complexity, and resource requirements are often immense so that multiple runs or ensembles of runs may not be practical.
- *No microtheory*. Often there is no basic theory underlying model, e.g., no Navier-Stokes equation.

4.3 What strategies can be employed?

The model evaluation strategies identified in the workshop (only some of which were actually used in the examples) included the following:

- *Comparing model output to real-world data.* MM5 precipitation forecasts were compared with 48-hour averages from rain gauge data. Stochastic CORSIM simulations were compared with observed queue lengths. Sometimes these comparisons were qualitative, that is, feature comparisons. For example, FIRETEC simulations showed wind gusts, fire-line shape and areas not completely burned, which were qualitatively similar to those observed in real wildfires and the immunology model predictions were borne out.
- *Comparing model output to experiments.* FIRETEC simulation output was compared to output from wind tunnel experiments and to controlled burns, where at least some of the site-specific conditions prior to the burn had been measured.
- *Comparing different models.* In Fovell's presentation, MM5 output without data assimilation was compared to model output using data assimilation. Perelson suggested developing independent implementations of the antigenic distance model and comparing results.
- *Comparing model to theory*. For example, the direction of flow of the main Atlantic and Pacific gyres must agree with the laws of physics governing fluids in a rotating system. This type of comparison is done more or less formally throughout model development and application.

- *Comparing model performance to experience/expert judgement.* Spillback appeared to be too great in traffic simulation, or queue times were too long in some runs. These comparisons are also done more or less formally for most models during development and application.
- *Varying resolution and physics* (including the parameterization of unresolved effects). Small-scale turbulence and cloud formation are subscale, parameterized processes in the mesoscale atmospheric model MM5. Alternative parameterizations might be considered. Output can also be compared across the three nested grids.
- *Comparing model output distributions across many runs* (statistical summaries) with data. For stochastic models such as CORSIM or the antigenic distance model, as well as for deterministic models for which input and boundary conditions are only statistically known, both the mean and the spread among model runs need to be compared with the available data.

4.4 What is the role for statistical concepts and tools, and where are the statistical gaps?

Not too surprisingly there were lots of ideas for the role of statistical concepts and tools. Gaps can be inferred from answers to the “what makes evaluation difficult” question, and some of the recurring “gap” themes are listed below.

Available tools include the following:

- Statistical techniques for sensitivity and uncertainty analysis. These continue to be a subject of very active research. Some new directions have recently been proposed by Kennedy and O’Hagan (2000).
- Statistical approximations to numerical code. Statistically equivalent models (SEMs) were mentioned by Schoenberg in the context of FIRETEC for assisting with inversion or sensitivity analysis of a model, and by Bickel as an alternative implementation of the antigenic distance hypothesis. They may also replace physical submodels within a large, complex computer model.
- Outlier analysis for detecting bugs and other anomalies.
- Various statistical tools for calibrating and improving models including combining data and model (e.g., nudging and data assimilation).
- Developing functionals of model output, which optimize discrimination among models or model parameterizations relative to given criteria.

- Statistical graphical techniques for visualization and statistical pattern recognition and imaging techniques to quantify differences in qualitative features.
- Experimental design for computer experiments and data collection, particularly in the presence of major practical constraints. Modeling the contribution of the uncertainty (biases) introduced by such constraints.
- Statistical techniques for tuning input parameters (model calibration).
- Adjoint methods, in particular using statistically equivalent models for the efficient approximation of adjoints and to quantify sensitivities to inputs.
- Statistical techniques to reduce dimensionality (principal components, other orthogonal decompositions such as wavelets, etc.)
- Analysis of covariance structure of observational data versus that of model predictions.

Some of the "gap" themes identified included bringing formalism to "eye ball" or "viewgraph" comparisons, and to statements such as "the simulation and real world pictures of the traffic flow *look alike*." A theory of multiscale phenomena—in particular techniques to quantify uncertainty when moving between scales (e.g. moving from finer local models to larger-scale models)—is needed. Better definitions and theory are needed for what is meant by *model uncertainty*. There is also a need for more clarity about the differences between model calibration and model evaluation, particularly when some of the available data are used for calibration. Better tools are needed for comparing competing models and discriminating between models.

In addition to these gaps, Greg McRae (MIT) identified the need to build deterministic models that deal with model uncertainty from the beginning. He maintained that "if uncertainty is crucial to the model, then putting it in the beginning is critical." McRae asserted that this approach "will lead to very different models" and that "physical scientists, applied mathematicians and statisticians must work together to do it."

5. WORKSHOP CONCLUSIONS AND NEXT STEPS

The presentations and discussions reinforced the observations that motivated the workshop. The diversity of the presentations emphasized that computer models are found in a variety of scientific fields and policy applications, and have many different formal structures. These models are often complex in the sense that they attempt to resolve a large number of relationships, many of which are highly non-linear, often with positive and negative feedback.

The workshop discussions underscored that current computer model evaluation practice is typically inadequate, sometimes grossly so. Possible explanations were identified as the enormous difficulty of the task, the inadequate resources, the need for new evaluation strategies and tools, and the incentive structure of the scientific community.

The workshop generated substantially more questions than answers, however it did much to focus the research issues. Many of these have been identified in the article. To summarize, computer model evaluation as well as the discipline of statistics will benefit from the invention and utilization of new techniques for model evaluation emerging from research in Bayesian methods, uncertainty quantification in deterministic models, designing field experiments to match computer experiments (and vice versa), data collection schemes, data reduction methods, data mining, and imaging and statistical visualization. However, workshop participants emphasized that in addition to the research, statisticians and applied mathematicians must meet the challenge of transferring these methodologies to the model developers and model users.

The final session of the workshop addressed the question "what next?" Many good suggestions were made, including the following.

- Develop a website for communication of the participants in this workshop and others interested in continuing the discussions.
- Conduct smaller workshops on specific aspects of model evaluation.
- Promote education among statisticians: probability and statistics that use real work examples for the modelers as well as science and engineering for the statisticians and mathematicians.
- Start collaborations, and develop an understanding of why some collaborations work better than others.
- Maintain and expand training opportunities for graduate students and post docs in statistics in settings like the national laboratories and the National Center for Atmospheric Research where computer model evaluation problems in multidisciplinary settings abound.
- Work to break down funding barriers for collaboration, e.g., modelers are reluctant to spend scare resources on statistical assistance, particularly when the worth of such collaborations has not yet been widely established.
- Support statisticians who can promote the computer model evaluation area at high levels within funding agencies.
- Develop a framework and consistent language to address evaluation techniques that the modeling community could use.

• Develop new and useful research in the area.

Finally, the most notable recommendation was that we **do something** to keep the energy and momentum generated during the workshop moving such that we begin to resolve the many and varied problems related to computer model evaluation. We hope that this article, the open questions raised, and the list of continued activities will keep us moving forward.

6. REFERENCES

BAYARRI, S. and BERGER, J. (1999). Quantifying Surprise in the Data and Model Verification. In *Bayesian Statistics* 6, (J.M. Bernardo, J.O. Berger, A.P. Dawid and A.F.M. Smith, eds.) 53-82. Oxford University Press, London.

BEYER, W. E. P., DEBRUIJN, I. A. (1998). WESTENDORP, R. G. J. and OSTERHAUS, A. D. M. E. *Vaccine* **16**, 1929-1932.

BOSSERT, J., REISNER, J. M., LINN R. R., WINTERKAMP J. L., SCHAUB R., and RIGGAN, P. J. (1998). Validation of Coupled Atmosphere-Fire Behavior Models. Preprints of the 14th Conference on Fire and Firest Meteorology, November 16-20, 1998, Luso-Coimbra, Portugal.

Box G.E.P. (1976) Scienec and statistics. Journal of the American Statistical Association, 71: 791-799.

BOX G.E.P. and DRAPER N. (1987) Empirical Model Building and Response Surfaces. J. Wiley, New York .

Brieman, L. (2001) Statistical Modeling: the two cultures. Statistical Science, 16: 199-231.

CLARK, T. L., RADKE L., COEN J., and MIDDLETON D., 1999: Analysis of small-scale convective dynamics in a crown fire using infrared video camera imagery. J Appl. Meteor., 38, (in Press)

CLICK, S. and ROUPHAIL, N. (1999). Lane Group Level Field Evaluation of Computer-based Signal Timing Models, Paper presented at the 78th Annual Meeting, TRB.

CORSIM USER'S MANUAL. (1997). FHWA, U.S. Department of Transportation, Office of Safety and Traffic Operation R&D, Intelligent Systems and Technology Division, McLean, VA.

EFRON B. and TIBSHIRANI R. (1993). Introduction to the bootstrap. Chapman and Hall, London.

GOLDBERG, D. E. (1989). Genetic Algorithms in Search, Optimization, and Machine Learning. Addison-Wesley, Reading.

HOSKINS, T. W., DAVIS, J. R., SMITH, A. J., MILLER, C. L. and Allchin, A. (1979) *Lancet* **i**, 33-35.

KIEFER J. and WOLFOWITZ J. (1952) Stochastic estimation of the maximum in a regression. Ann. Math. Stat. 462-466.

KEITEL, W. A., CATE, T. R., COUCH, R. B., HUGGINS, L. L. and HESS, K. R. (1997) *Vaccine* **15**, 1114-1122.

KENNEDY, M. AND O'HAGAN, A. (2000). Bayesian Calibration Of Computer Models. J. Royal Statistical Society, Series B **63**, 425-450

KUSHNER H., and LIN G. (1997). Stochastic Approximation algorithms and Applications. Springer-Verlag Inc., New York .

LINN, R. R. (1997). Transport Model for Prediction of Wildfire Behavior, Los Alamos National Laboratory Scientific Report: LA13334-T.

MCKAY, M. D., BECKMAN, R. J. and CONOVER, W. J. (1979). Comparison of three methods for selecting input variables in the analysis of output from a computer code. Technometrics 21, 239-245.

MILLER, R. G. (1966). Simultaneous statistical inference. McGraw Hill, New York

PERELSON, A. S. and OSTER, G. F. (1979). *J. Theor. Biol.* **81**, 645-670.

SACKS, J., SCHILLER, S. B. and WELCH, W. J. (1989). Designs for computer experiments (with discussion). Technometrics 31, 41-47

SCHOENBERG, F., BERK, R., FOVELL, R., LI, C., LU, R., and WEISS, R. (2001). Approximation and Inversion of a Complex Meteorological System via Local Linear Filters. J. Appl. Meteorology, to appear.

SMITH, D. J., FORREST, S., ACKLEY, D. H. and PERELSON, A. S. (1999). Proc. Natl. Acad. Sci. USA **96**, 14001-14006.

SMITH, D. J., FOREST, S., ACKLEY, D. H. and A. S. PERELSON (2000). Variable efficacy of repeated annual influenza vaccination, PNAS. 96 14001-14006.

STORCH, H. von and NARVARRA, A. (1999). Analysis of Climate Variability: Applications and Statistical Techniques, Springer-Verlag.

ZEIGLER, B. (1976). Theory of modelling and simulation, John-Wiley, New York.